Phase transitions in the spinless Falicov-Kimball model with correlated hopping

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Abstract

The canonical Monte-Carlo is used to study the phase transitions from the low-temperature ordered phase to the high-temperature disordered phase in the two-dimensional Falicov-Kimball model with correlated hopping. As the low-temperature ordered phase we consider the chessboard phase, the axial striped phase and the segregated phase. It is shown that all three phases persist also at finite temperatures (up to the critical temperature τ_c) and that the phase transition at the critical point is of the first order for the chessboard and axial striped phase and of the second order for the segregated phase. In addition, it is found that the critical temperature is reduced with the increasing amplitude of correlated hopping t' in the chessboard phase and it is strongly enhanced by t' in the axial striped and segregated phase.

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1 Introduction

The Falicov-Kimball model is one of the simplest yet most versatile models of strongly correlated electron systems on the lattice [1]. The model describes a two-band system of localized f electrons and itinerant d electrons with the short-ranged f-d Coulomb interaction U. The Hamiltonian is

$$H_0 = \sum_{ij} t_{ij} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i, \tag{1}$$

where f_i^+, f_i are the creation and annihilation operators for an electron in the localized state at lattice site i with binding energy E_f and d_i^+, d_i are the creation and annihilation operators for an electron in the conduction band. The conduction band is generated by the hopping matrix elements t_{ij}, which describe intersite transitions between the sites i and j. Usually it is assumed that $t_{ij} = -t$ if i and j are nearest neighbours and $t_{ij} = 0$ otherwise (the conventional Falicov-Kimball model).

The model has been used in the literature to study a great variety of many-body effects in metals, of which valence and metal-insulator transitions, charge-density waves and electronic ferroelectricity are the most common examples [2, 3, 4, 5]. It has been applied to a variety of lattices, one [6, 7], two [8, 9, 10], three [11], and infinite dimensional [12], and occasionally to small clusters [13, 14, 15]. Exact results are available in very few instances [12, 16, 17, 18] and general theorems have been proved for special cases [9, 19]. In spite of the existence of an analytic solution in $d = \infty$ dimension [12, 20] and an impressive research activity in the past, the properties of this seemingly simple model are far from being understood, especially for nonzero temperatures. For example, it is well known [21] that the ground-state phase diagram of the model exhibits a rich spectrum of charge ordered phases including various types of axial and diagonal striped phases, the chessboard phase, the segregated phase, etc., but only a little is known about the temperature stability of these phases [22, 23]. Similarly, only a little is known about the type of phase transitions from the ground-state ordered phases to the high-temperature disordered phase [24]. From this point of view the most explored phase from the above mentioned ones is the chessboard phase that is the ground state of the model at the half-filled band case ($E_f = 0$, $N_f = N_d = L/2$, where L is the number of

lattice sites). For this case there exists the exact proof [9] of existence the phase transition from the low-temperature ordered phase (the chessboard phase) to the high-temperature disordered phase at finite critical temperature τ_c (for dimensions $d \geq 2$) that strongly depends on the local Coulomb interaction U. In addition, the numerical simulations within the grand-canonical Monte-Carlo showed that the phase transitions are of the first order for small and intermediate values of the Coulomb interaction U and of the second order for strong interactions [24, 25]. In the current paper we extend the numerical study of the temperature induced phase transitions also on the case of phase segregated and striped phases. Moreover, we consider here a more general situation

$$H = H_0 + H_{t'} \tag{2}$$

with the correlated hopping term

$$H_{t'} = t' \sum_{\langle i,j \rangle} (f_i^+ f_i + f_j^+ f_j) d_i^+ d_j \ , \tag{3}$$

that represents a much more realistic description of electron hopping in rare-earth compounds [26]. As was shown in our previous papers [27, 28] this term has strong effect on the formation of charge ordering in the ground state and therefore it should be taken into account in the correct description of electronic correlations in rare-earth materials. In particular, we have found that already relatively small values of the correlated hopping term lead to a stabilization of new types of charge ordering, even in the half-filled band case, where the ground state at $t' = 0$ is the chessboard phase for all nonzero U. The comprehensive ground-state phase diagram of the two-dimensional half-filled Falicov-Kimball model with the correlated hopping in the $t' - U$ plane is presented in [27]. It consists of three different phases, and namely (i) the chessboard phase located in the central region of the phase diagram along the U axis, (ii) the axial striped phase located below ($U > 0$) and above ($U < 2$) the chessboard phase, and (iii) the segregated phase located above the axial ($U < 2$) and chessboard ($U > 2$) phase. Since these phases represent the most prominent examples of charge ordering observed experimentally in strongly correlated materials, like cuprates, nickelates and cobaltates, we have decided to perform exhaustive numerical studies of the half-filled Falicov-Kimball model with the correlated hopping with a goal to answer the questions about the temperature stability of these phases

and the type of phase transitions from the low-temperature ordered phases to the high-temperature disordered one.

2 Method

Since in this spinless version of the Falicov-Kimball model with correlated hopping the f-electron occupation number $f_i^+ f_i$ of each site i commutes with the Hamiltonian (2), the f-electron occupation number is a good number, taking only two values: $w_i^f = 1$ or 0, according to whether or not the site i is occupied by the localized f electron. Therefore the Hamiltonian (2) can be written as

$$H = \sum_{\langle i,j \rangle} h_{ij}(w^f) d_i^+ d_j \tag{4}$$

where $h_{ij}(w^f) = \widetilde{t}_{ij}(w^f) + U w_i^f \delta_{ij}$ and

$$\widetilde{t}_{ij}(w^f) = t_{ij} + t'_{ij}(w_i^f + w_j^f). \tag{5}$$

Thus for a given f-electron configuration w^f=$\{w_1^f, w_2^f, \ldots, w_L^f\}$, defined on the two-dimensional lattice of L sites, the Hamiltonian (2) is the second-quantized version of the single-particle Hamiltonian $h(w^f)$, so the investigation of the model (2) is reduced to the investigation of the spectrum of h for different configurations of f electrons. Since we are interesting in the half-filled band case, where both the total number of f and d electrons are fixed to $L/2$, the numerical calculations at nonzero temperatures are done exclusively in the canonical ensemble. In this formalism the partition function and the internal energy corresponding to the model Hamiltonian (2) can be written as:

$$Z = \sum_{w^f, w^d} e^{-E/\tau}, \qquad E = \sum_i \varepsilon_i(w^f) w_i^d \tag{6}$$

$$\langle E \rangle = \sum_{w^f, w^d} E e^{-E/\tau}, \tag{7}$$

where $\tau = k_B T$ and the summation goes over all possible $L!/N_f!(L-N_f)!$ distributions w^f of f electrons on L lattice sites and $L!/N_d!(L-N_d)!$ distributions w^d of d electrons on L single-particle energy levels ε_i corresponding to $h(w^f)$. In the next step the summation over all f and d distributions is replaced by the Monte-Carlo summation with the statistical weight $e^{-E/\tau}/Z$.

To identify the transition temperatures from the low-temperature ordered phases to the high-temperature disordered phase and the type of the phase transition we have calculated numerically the specific heat $C = (\langle E^2 \rangle - \langle E \rangle^2)/(L\tau^2)$, the thermal average of the f-electron occupation $w_s = \langle w^f \rangle$ and the energy distribution $P(E)$. The numerical calculations are done exclusively at $U = 0.5$, since the ground-state phase diagram exhibits the richer spectrum of solutions in the weak and intermediate coupling regions in comparison to the strong coupling limit.

3 Results and discussion

To verify the ability of our method to describe the phase transitions at finite temperatures we have started with the conventional two-dimensional Falicov-Kimball model ($t' = 0$) at half-filling. As was mentioned above, the physical picture of temperature-induced phase transitions within this relatively simple model is well understood at present. For all finite Coulomb interaction $U > 0$ the ground state of the model is the chessboard phase that persists up to critical temperature $\tau_c(U)$, where the system undergoes the phase transition to the homogeneous phase. The phase transition is of the first order for $U < 1$ and of the second order for $U > 1$ [24]. Our numerical results obtained within the canonical Monte-Carlo method for C, w_s and $P(E)$ fully confirm this picture (see Fig.1). The specific heat curves exhibit a sharp low-temperature peak at $\tau_c \sim 0.028$ that is connected obviously with the phase transition from the chessboard phase to the homogeneous phase, as can be seen from the behaviour of the average f-electron occupation w_s for temperatures slightly lower or slightly higher than τ_c. Moreover, the energy distribution function $P(E)$ exhibits an apparent two-peak structure near the critical point τ_c (it can be considered as a superposition of two Gaussians), what in accordance with the theory of Challa, Landau and Binder [29] points on the first order phase transition at τ_c.

Let us now discuss how this picture is changed when the correlated hopping term is added. Firstly, we have examined the case of small values of $|t'|$ for which the ground state of the model is still the chessboard phase [27]. The typical examples of C, w_s and $P(E)$ from the positive and negative region of t' are displayed in Fig. 2 and Fig. 3 for $t' = -0.3$ and $t' = 0.3$. One can see that the correlated hopping term

(in the limit of small $|t'|$) does not change qualitatively the picture of temperature induced phase transitions found for $t' = 0$. For both, positive and negative t', there is the first order phase transition from the low-temperature ordered phase to the high-temperature disordered one, similarly as for $t' = 0$, and the only difference between these cases is that the correlated hopping term reduces slightly the critical temperature τ_c of the phase transition.

Therefore, in the next step we have turned our attention to the physically much less explored type of configurations, and namely, the axial striped configurations that are ground states of the Falicov-Kimball model for the intermediate values of t' ($|t'| \sim 0.5$). Note, that for the axial striped phase even the fundamental question concerning the temperature stability of this phase has been not answered till now. This is caused by the fact that it is very difficult to find this phase in the pure form. For example, in the conventional Falicov-Kimball model ($t' = 0$) the axial striped phases are stable for a relatively wide range of model parameters [21], but only in mixtures with other phases (e.g., the empty configuration). In addition, strong finite-size effects have been observed on the stability of these mixtures and therefore it is practically impossible to do any conclusions concerning their stability at finite temperatures from the numerical calculations on finite clusters. However, in the Falicov-Kimball model with correlated hopping the axial striped phase exists in the pure form for wide range of model parameters t' and U, the finite-size effects on the stability of this phase at $\tau = 0$ are negligible, and so the corresponding numerical study of the temperature stability of the axial striped phase can be performed straightforwardly.

In Fig. 4 and Fig. 5 we present our canonical Monte-Carlo results for C, w_s and $P(E)$ obtained for two different values of t' ($t' = 0.5$ and $t' = 0.55$) from the region where the ground-state of the model is just the axial striped phase. Again, the specific heat curves exhibit the sharp low-temperature peak, the existence of which indicates the phase transition form the axial striped phase to the homogeneous phase. This was verified independently by calculating the average f-electron occupation w_s and the energy distribution $P(E)$ near the transition point τ_c, that clearly demonstrate the presence of the first order phase transition at τ_c. Since the critical temperature τ_c of the phase transition for both values of t' shifts to smaller values with increasing L, we have performed a detailed finite-size scaling analysis of the $\tau_c(L)$ dependence

to exclude a possibility that τ_c vanishes in the thermodynamic limit $L \to \infty$. The resultant $\tau_c(L)$ dependencies are plotted as insets in Fig. 4 and Fig. 5. It is seen obviously that the critical temperatures τ_c for both $t' = 0.5$ and $t' = 0.55$ persist also in the thermodynamic limit, what means that the axial striped phase remains stable also at finite temperatures. In addition, our numerical results show that the critical temperatures for the axial striped phase are considerably higher in comparison to the critical temperatures for the chessboard phase. The same behaviour we have observed also for negative values of t' ($t' = -0.7$), however the critical temperature in this case was only slightly larger than one corresponding to $t' = 0$.

With increasing t' the half-filled Falicov-Kimball model with correlated hopping exhibits (at $\tau = 0$) the phase transition from the axial striped phase to the segregated phase [27] that takes place at $t' \sim 0.6$. Since the chessboard phase as well as the axial striped phase are both insulating and the segregated phase is metallic [27], one can expect a fully different thermodynamic behaviour of the model for the last case. To verify this conjecture we have performed an exhaustive numerical studies of the temperature dependence of C, w_s and $P(E)$ for $t' = 1$. This study is important also from this point of view that the thermodynamic of the metallic phase has been examined till now only in a few cases [23, 30], while for the insulating phase (usually the chessboard phase) there is a number of analytical and numerical results [9, 31, 32].

The results of our numerical calculations obtained for the specific heat C are shown in Fig. 6. To reveal the finite-size effects the calculations for C have been done on several different clusters of L=6 $\times$ 6, 8 $\times$ 8, 10 $\times$ 10, 12 $\times$ 12 and 16 $\times$ 16 sites. We have found that the specific heat curves, in the low-temperature region, strongly depends on the cluster sizes, and therefore a very careful analysis has to be performed to find the correct behaviour of the model in the thermodynamic limit $L \to \infty$. On small finite clusters ($L = 6 \times 6$ and $L = 8 \times 8$) the specific heat exhibits only one-peak structure in the low-temperature region ($\tau \sim 0.15$). With the increasing cluster size L an additional peak is stabilized at slightly higher temperatures ($\tau \sim 0.23$), while the first peak is gradually suppressed and probably fully disappears in the thermodynamic limit. The behaviour of the average f-electron occupation shows (see Fig. 6) that the second peak in the specific heat corresponds to the phase transition from the low-temperature ordered (segregated) phase to the

high-temperature disordered phase.

The nature of this phase transition is, however, different in comparison to previous cases. While the energy distribution function $P(E)$ is double peaked for the chessboard and the axial striped phase near the transition temperature τ_c (the first order phase transition), $P(E)$ exhibits the single-peak structure for the segregated phase, what points on the second order phase transition at τ_c. Comparing the thermodynamic behaviour of the model in the chessboard, axial striped and segregated region one can find two other important differences, and namely, (i) the critical temperature of the second order phase transition is approximately ten times higher than the critical temperatures of the first order phase transitions, and (ii) the specific heat (in the low-temperature region) decreases exponentially for the chessboard and axial striped phase, while in the segregated phase the specific heat $C(\tau)$ seems to have the linear behaviour indicating the Fermi-liquid behaviour for $\tau < 0.08$ (see the inset in Fig. 6a). The observation of the linear contribution to the specific heat in the low-temperature region ($\tau < 0.08$) is consistent with behaviour of the average f-electron occupation in this region (see Fig.6c). One can see, that despite the increasing temperature (from 0 to 0.08) the f-electrons preferably occupy only one half of the lattice leaving another part empty. Due to the on-site Coulomb interaction between the f and d electrons, the itinerant d electrons occupy preferably the empty part of lattice, where they can move as free particles yielding the linear contribution to the specific heat.

In summary, we have studied the phase transitions from the low-temperature ordered phase to the high-temperature disordered phase in the two-dimensional Falicov-Kimball model with correlated hopping using the canonical Monte-Carlo. As representative examples of low-temperature ordered phases we have chosen the chessboard phase, the axial striped phase and the segregated phase. It was shown that all three phases persist up to critical temperature τ_c and that the phase transition at the critical point is of the first order for the chessboard and axial striped phase and of the second order for the segregated phase. In addition, we have found that the critical temperature is reduced with the increasing amplitude of correlated hopping t' in the chessboard phase and it is strongly enhanced by t' in the axial striped and segregated phase.

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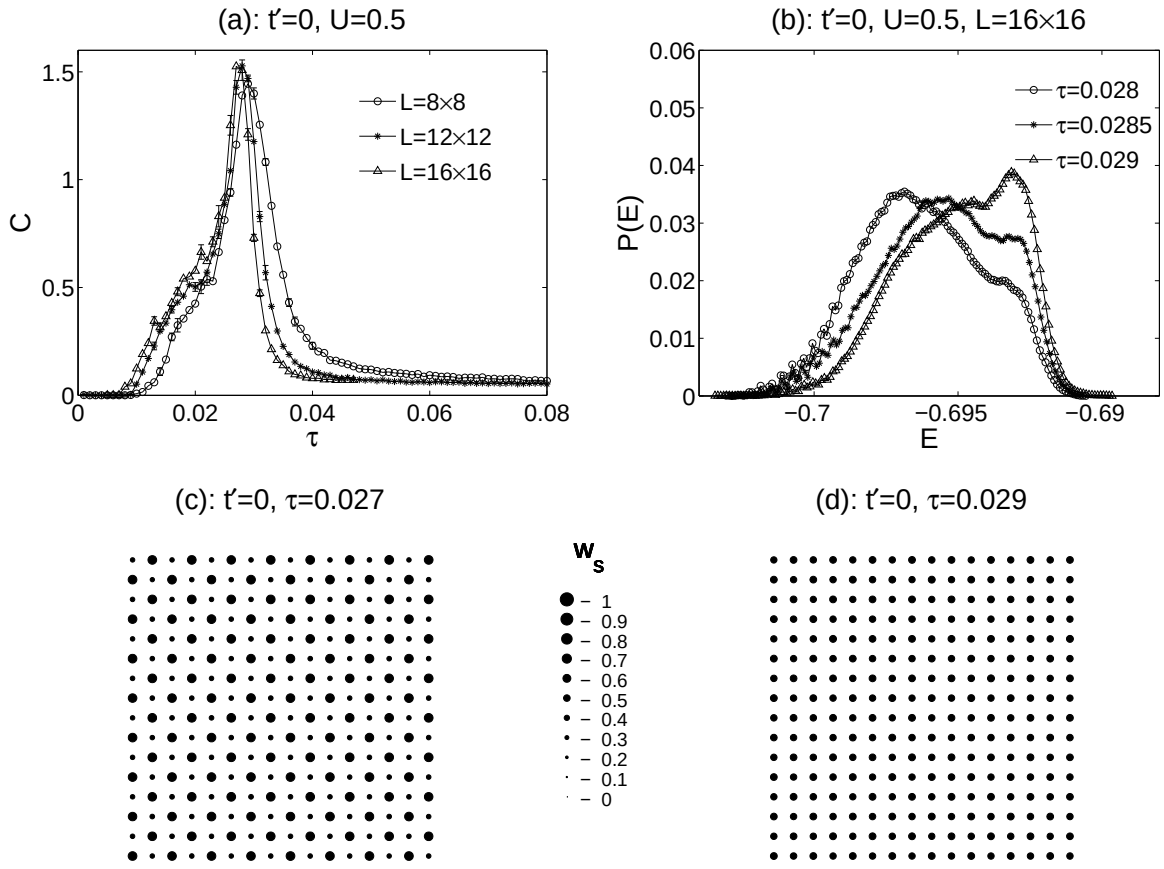

Figure 1: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-d) for the conventional Falicov-Kimball model ($t' = 0$) in two dimensions.

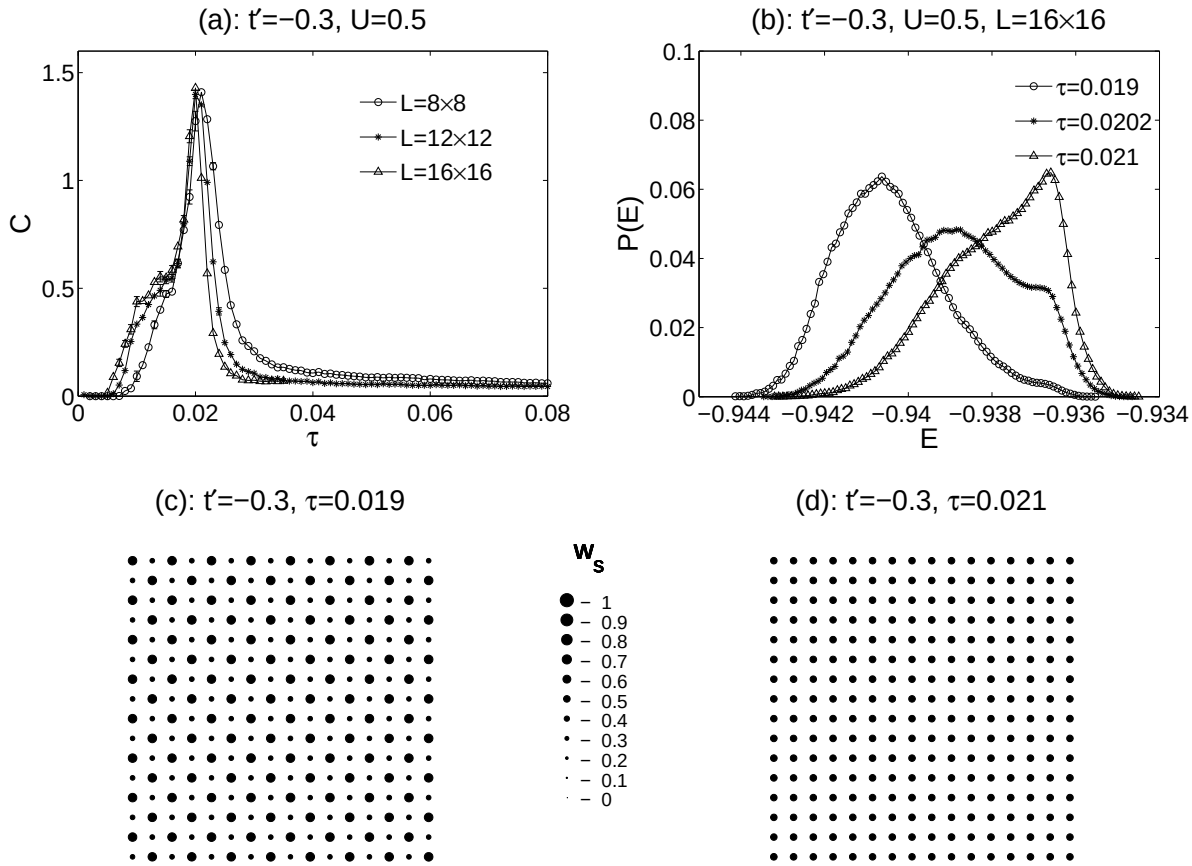

Figure 2: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-d) for the two-dimensional Falicov-Kimball model with correlated hopping $t' = -0.3$.

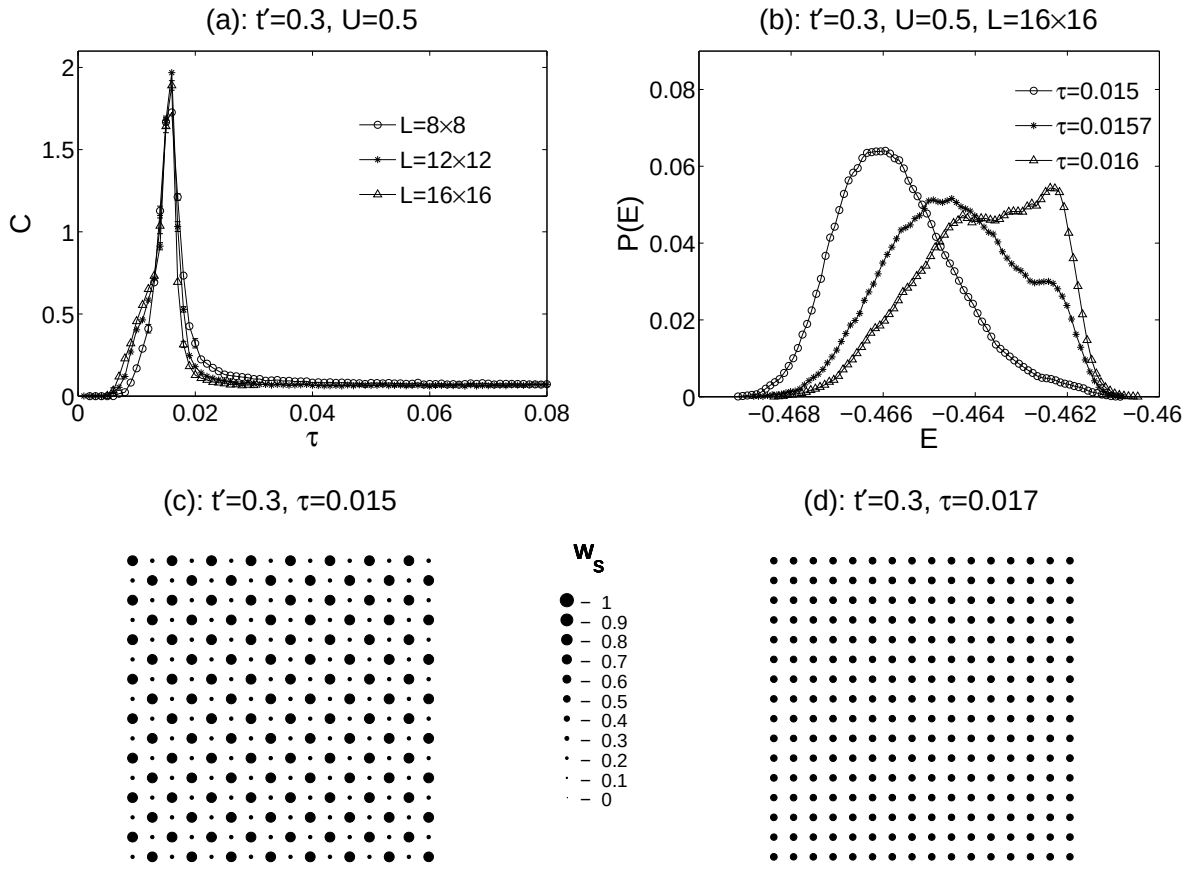

Figure 3: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-d) for the two-dimensional Falicov-Kimball model with correlated hopping $t' = 0.3$.

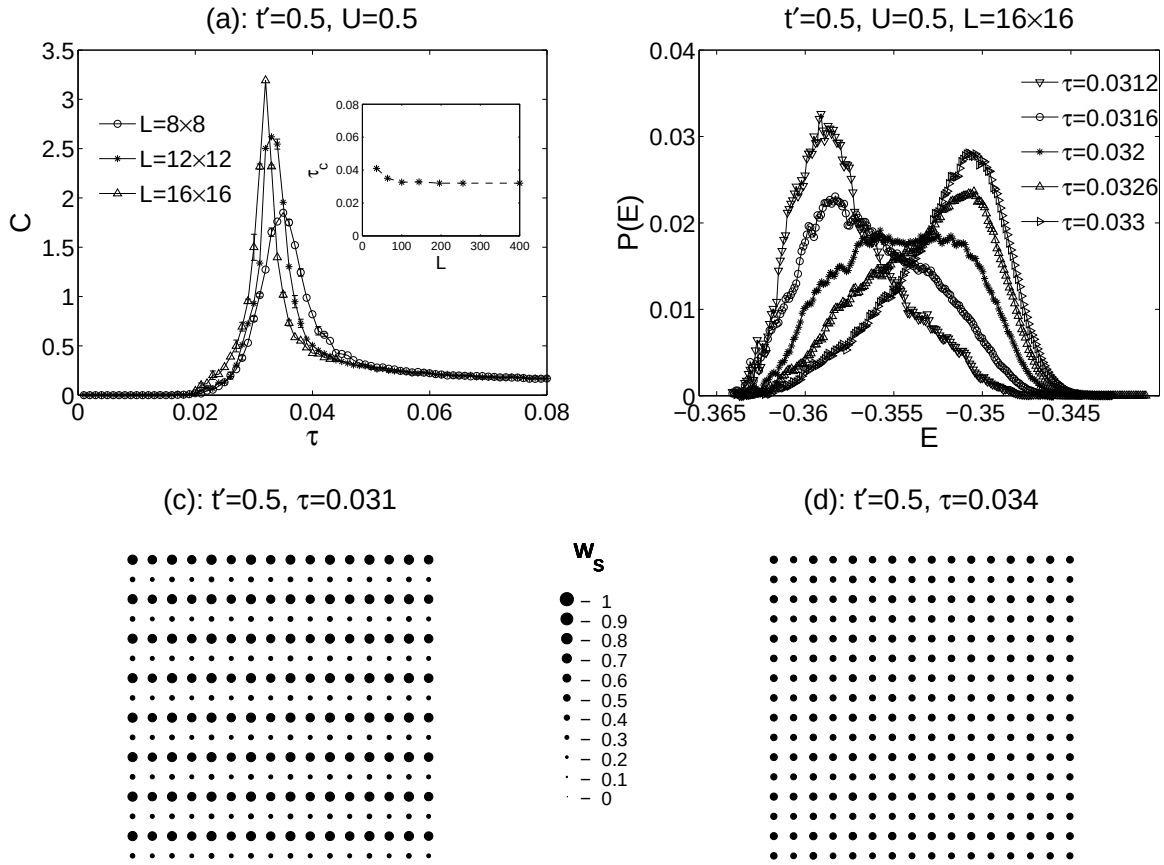

Figure 4: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-d) for the two-dimensional Falicov-Kimball model with correlated hopping $t' = 0.5$. The inset shows the critical temperature τ_c as a function of the cluster size L.

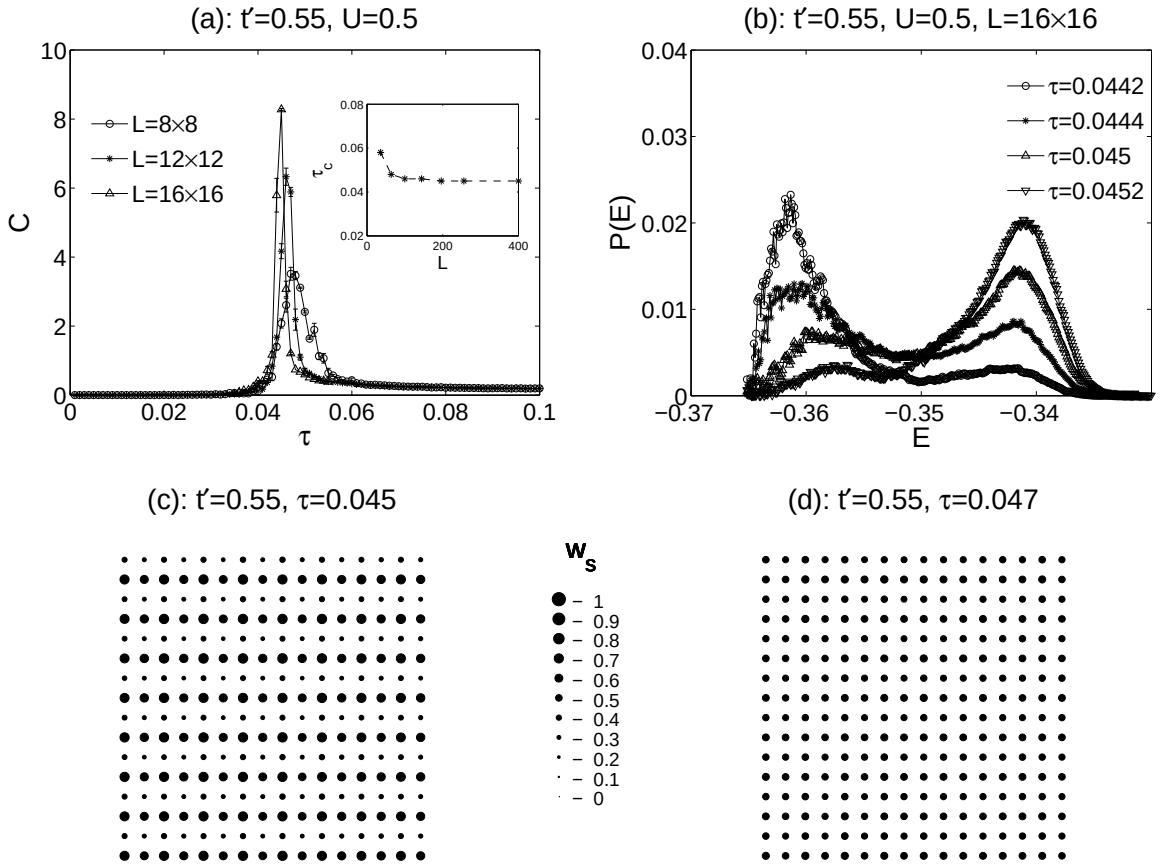

Figure 5: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-d) for the two-dimensional Falicov-Kimball model with correlated hopping $t' = 0.55$. The inset shows the critical temperature τ_c as a function of the cluster size L.

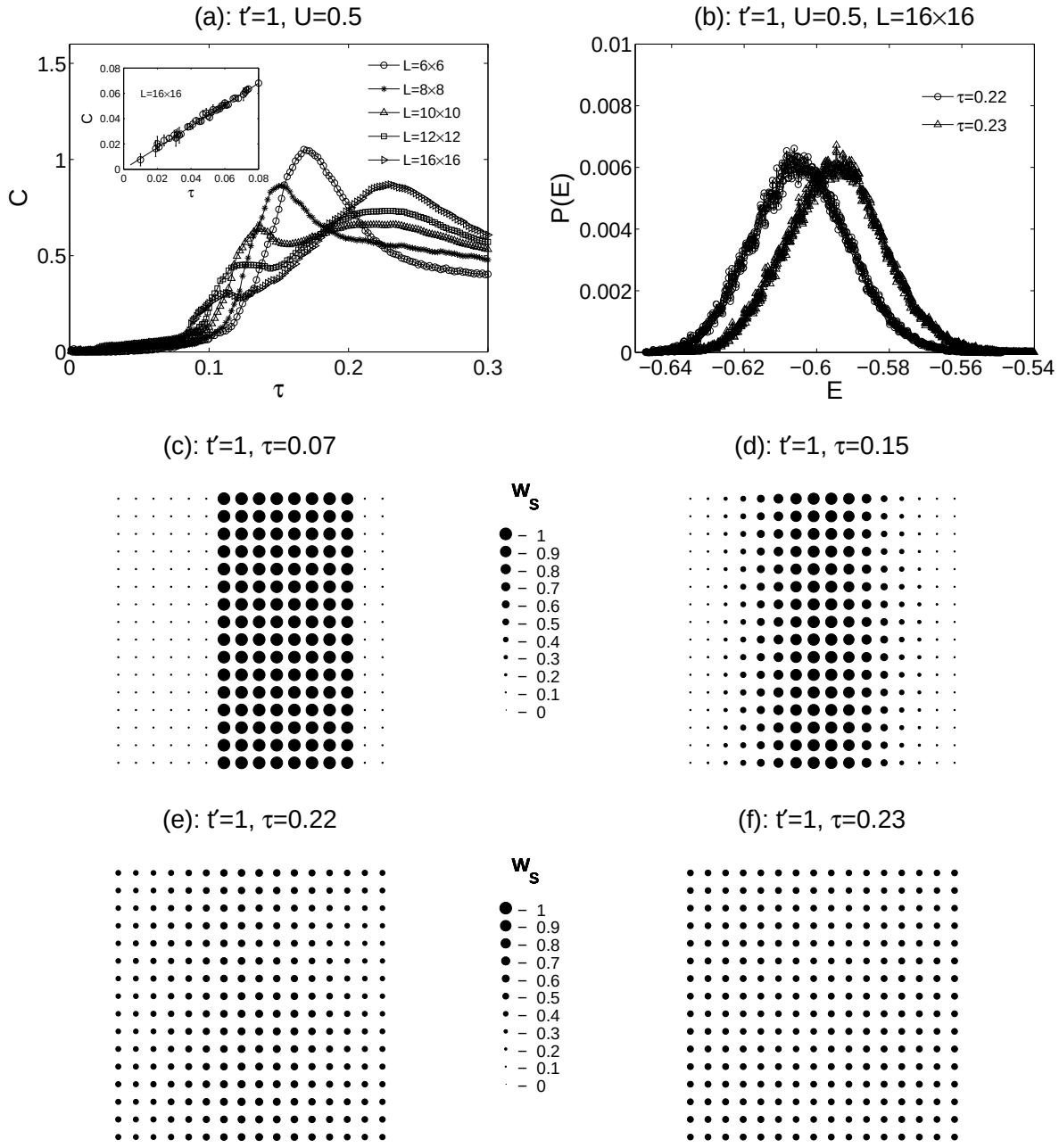

Figure 6: The specific heat (a), the energy distribution (b) and the thermal average of the f-electron occupation (c-f) for the two-dimensional Falicov-Kimball model with correlated hopping $t' = 1$. The inset shows the specific heat C in the low-temperature region for $L = 16 \times 16$.